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PARAMETER OPTIMISATION AND SENSITIVITY OF AN EUTROPHICATION SIMULATOR

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ABSTRACT

Water quality management of freshwater ecosystems requires decisions which are based on suitable simulation models. In this context, the setting up of parameter values and initial conditions is of high importance. Therefore, the eutrophication simulator CEUS was investigated by sensitivity analysis. For eutrophication management those parameters are of special interest which is connected with algal growth.. The output of CEUS was found to be most sensitive for parameters of phytoplankton growth. Another group of sensitive parameters could be identified describing nutrient cycles within the water body. In opposite of that, the interactions within in a food chain was less sensitive. The importance of parameters is visualized by ranking with Hasse diagram technique.

Index Terms – Modelling, parameter optimisation, parameter sensitivity, eutrophication, water quality management

1. INTRODUCTION

Management options for water quality management, especially eutrophication control will be obtained by scenario analyses with changing parameter values. To get suitable simulation results setting up of parameter values and initial conditions is of high importance. For parameterisation four different approaches can be taken into account [7]:

1. A preliminary estimate is obtainable from laboratory and field observations of processes and effects by means of correlation analysis or by parameter estimation techniques.
2. Combinations of parameters in keeping with a modelled situation may be obtained by means of estimation from parameter optimization techniques.
3. Estimates of parameters of a simulation model are obtained by sensitivity analysis according to major parameter changes Δp .

4. Analytical sensitivity analysis by computation of partial derivatives of state variables u_j to parameters: $S(p_i) = \partial u_j / \partial p_i$. This differential method of sensitivity analysis is based on linearization around the nominal solution by numerical or graphical procedures.

Optimization procedures refer to goal functions including output variables of a model. One problem of parameter optimisation is the determination of suitable goal functions according to the model output. Another problem is the existence of a global minimum during search. In opposite of engineering or logistics models ecological models are often similarly optimal for several parameter combinations [6]. In some cases process conditions and restrictions will be superimposed on parameter and/or state variables and other balance terms. Because of the multi-lateral complexity of environmental systems there is no objective procedure for determining the most appropriate parameter combination.

The problem of parameter optimisation can be described related to a model's quality and accuracy [5]. Under the prerequisite of well-founded initial parameter settings a higher accuracy will be obtained by iterative optimization techniques [4]. Then, parameter sensitivity according to output variables gives information how to select and weight the parameters and on which range and accuracy they have to be treated.

2. THE SIMULATOR CEUS

A MATLAB based stationary 1D eutrophication simulator for freshwater ecosystems was developed by [3] and coupled with an optimisation tool ISSOP [4]. The model equations are given below. A detailed description and explanation of model variables and parameters will be found in [3].

Phytoplankton, A (mg CHA/l):

$$\frac{dC_A}{dt} = \frac{Q}{V} \cdot (C_{A,IN} - C_{A,OUT}) - UA \cdot f \cdot C_A + GROW - FRZ \cdot CR \cdot C_Z \cdot C_A - RESP \cdot T \cdot C_A$$

Orthophosphate Phosphorus, P (mg P/l):

$$\begin{aligned} \frac{dC_P}{dt} = & \frac{Q}{V} \cdot (C_{P,IN} - C_{P,OUT}) + \frac{1}{4} \cdot \frac{dC_{P,SED}}{dt} - GROW \\ & + FRZ \cdot CR \cdot C_Z \cdot C_A \cdot \left((1 - AZP) \cdot \frac{K_{SA}}{K_{SA} + C_A} \right) + RESP \cdot T \cdot C_A \end{aligned}$$

Ammonium Nitrogen, NH₄-N (mg N/l):

$$\frac{dC_{NH4}}{dt} = \frac{Q}{V} \cdot (C_{NH4,IN} - C_{NH4,OUT}) - FA1 \cdot FUP \cdot GROW + B3 \cdot C_{NORG,IN} - B1 \cdot C_{NH4}$$

Nitrate Nitrogen, NO₃-N (mg N/l):

$$\frac{dC_{NO3}}{dt} = \frac{Q}{V} \cdot (C_{NO3,IN} - C_{NO3,OUT}) - FA1 \cdot (1 - FUP) \cdot GROW + B1 \cdot C_{NH4}$$

Zooplankton, Z (mg C/l):

$$\frac{dC_Z}{dt} = \frac{Q}{V} \cdot (C_{Z,IN} - C_{Z,OUT}) - MORT \cdot C_Z \cdot T + FRZ \cdot CR \cdot C_Z \cdot C_A \cdot q_{C,CHA} \cdot AZP \cdot \frac{K_{SA}}{K_{SA} + C_A}$$

Phosphorus Remobilisation, PSED (mg P/l):

$$\frac{dC_{P,SED}}{dt} = \phi h_s \cdot \left(-D_{p,T} \cdot \frac{1}{1 - \ln(\phi^2)} \cdot \frac{C_p - C_{P,SED}}{h_s \phi} + \Theta \cdot \frac{C_{EA,POWA,crit} - C_{EA,POWA}}{C_{EA,POWA,crit}} K_{Fe,T} \cdot C_{Fe,POWA} \cdot q_{D,Fe} \right)$$

for $\Theta = 1$, for $CEA,POWA \leq CEA,POWA,crit$
and $\Theta = 0$, for $CEA,POWA > CEA,POWA,crit$.

3. SENSITIVITY OF PARAMETERS

Estimating sensitivity to external parameters, those connected with driving variables or site constants, a picture is getting how a given freshwater ecosystem would behave under changing environmental conditions, e.g. global warming. In fig. 1 direct and indirect relationships of model parameters to model variables can be seen.

The rates GROW_{MAX}, KSP and KSNO₃ directly influence the overall phytoplankton biomass concentration and the concentration of the nutrients nitrogen and phosphorus. The nitrogen fraction of algae biomass FA1 and the ammonification rate B3 directly affect the nitrogen compounds ammonium and nitrate. The half saturation rate KSA appears in the equation of zooplankton and in the phosphorus equation. The filtration rate FRZ as well as the respiration rate RESP has a direct influence food chain processes.

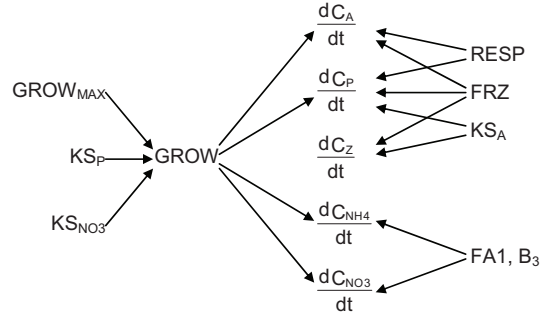


Figure 1 Direct and indirect relationships between model parameters and model variables

Parameter optimisation of a complex multi parameter system is a non-solvable task. Especially, the inadequate amount of real data, including short-term and long-term ecological changes, restricts the model quality and therefore the decisions based simulation runs. In practice, valuable results of optimisation procedures applied to environmental simulation models will be obtained for a limited number of parameters only.

For the above given rate constants reference values are presented in tab. 1 where p*up is twice the reference value (200%·p*) and p*low corresponds to a tenth of it (10%·p*).

Table 1 Reference values of parameters

Parameter p	Ref. val. p*	p*low	p*up
GROW _{MAX}	5	0.5	10
KSP	30	3	60
KSNO ₃	0.1	0.01	0.2
KSA	0.06	0.006	0.12
FRZ	0.1	0.01	0.2
FA1	50	5	100
B3	0.02	0.002	0.04
RESP	1.4·10 ⁻⁵	1.4·10 ⁻⁶	2.8·10 ⁻⁵

On the base of this reference values any parameter p has been varied in the interval [p*low; p*up] by the equation

$$\Delta x = \max_{p,t} |xp(t) - xp^*(t)|.$$

Hereby denotes $xp(t)$ the value of model variable x at time t for a specific parameter value p .

4. RESULTS AND DISCUSSION

Ranking these rate constants according to variations of phytoplankton biomass ΔCHA , to

orthophosphate phosphorus concentrations $\Delta\text{-PO}_4\text{-P}$, to ammonia nitrogen concentrations $\Delta\text{NH}_4\text{-N}$, and to nitrate nitrogen concentrations $\Delta\text{NO}_3\text{-N}$ the four variables show a partition of the parameter set into three groups:

1. Group G1 = {GROWMAX, FA1, KSP} high sensitivity,
2. Group G2 = {KSNO₃, B3} medium sensitivity,
3. Group G3 = {KSA, FRZ, RESP} low sensitivity.

In order to summarise rankings of multiple variables partial ordering is one way to visualise ordinal relationships and avoiding subjective weighting functions by means of Hasse diagrams [2]. Fig. 2 summarises the results in a Hasse diagram. It shows the sensitivity of the variables CHA, o-PO₄-P, NH₄-N and NO₃-N to the parameters of groups G1 to G3.

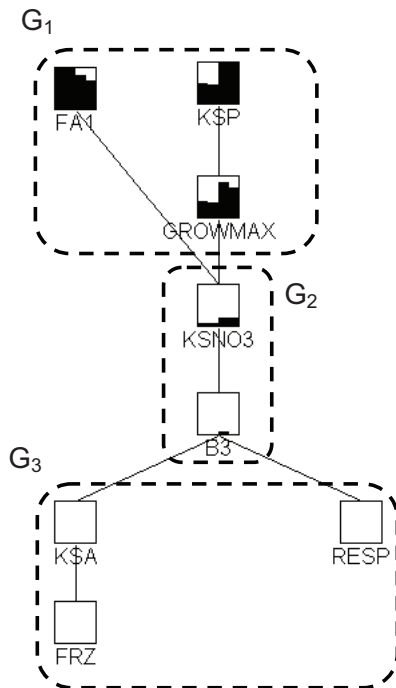


Figure 2 Hasse diagram of groups of parameter sensitivity (Bars: CHA, o-PO₄-P, NH₄-N, NO₃-N)

Concerning the variable CHA the parameter FA1 (nitrogen fraction of phytoplankton biomass) has the highest influence on the total amount of phytoplankton biomass. This is in accordance with the extremely increase of algal biomass due to growth of cyanobacteria in late summer and early fall. It corresponds also with rate GROW_{MAX} for ammonia nitrogen and nitrate nitrogen. The result will be confirmed by the in-

tensity of the rate constant KSNO₃ of group G2. Fig. 3 shows detailed information of the tendency of state variables by changing parameter values.

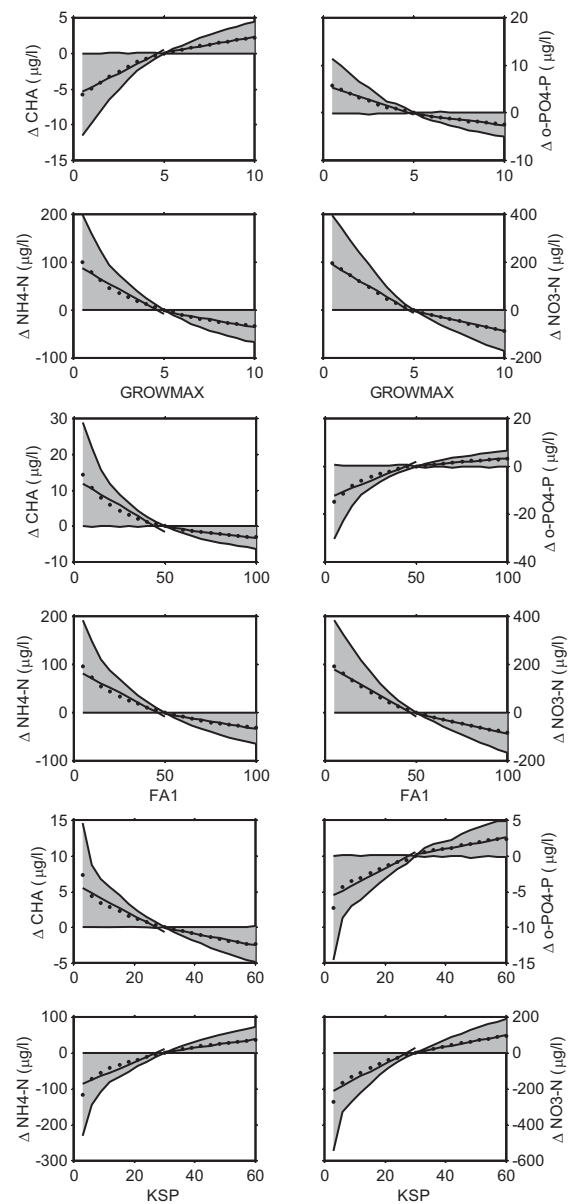


Figure 3 Sensitivity of variables CHA, o-PO₄-P, NH₄-N and NO₃-N to the parameters of group G1

For increasing values of GROW_{MAX} the variable CHA increases only. All nutrient variables show a decreasing behaviour for increasing parameter values which is in accordance with experimental observations. The rate FA1 has a strong negative influence to biomass production. With decreasing nitrogen parameter values the amount of phytoplankton biomass decreases while the phosphorus level shows an increasing trend for the Lower Havel River basin.

In fig. 4 the sensitivity of the variables to the parameters of group G2 = {KSNO₃, B3} is represented.

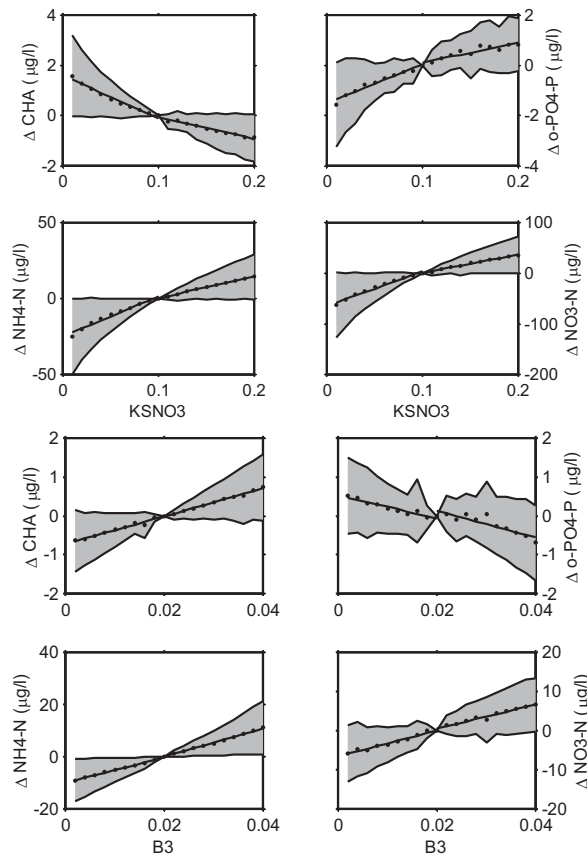


Figure 4 Sensitivity of variables CHA, o-PO₄-P, NH₄-N and NO₃-N to the parameters of group G2

The parameter KSNO₃, the half-saturation constant for nitrate nitrogen, which is a part of the growth function GROW influences the growth of phytoplankton. The function GROW is a negative term in all the nutrient equations, but a positive term in the phytoplankton equation. Therefore, one gets for increasing values of KSNO₃ decreasing algal concentrations. Another effect can be observed for increasing parameter values of the ammonification rate B3. A higher intensity of the internal ammonification process leads to higher phytoplankton concentrations. Therefore, the influence of phosphate phosphorus onto phytoplankton will be diminished which results in decreasing values of orthophosphate phosphorus.

From fig. 5 a constant or a slight positive or negative influence of the parameters KSA, FRZ and RESP onto the state variables considered is observed. This is in accordance with experimental results of laboratory investigations for different algal species [1].

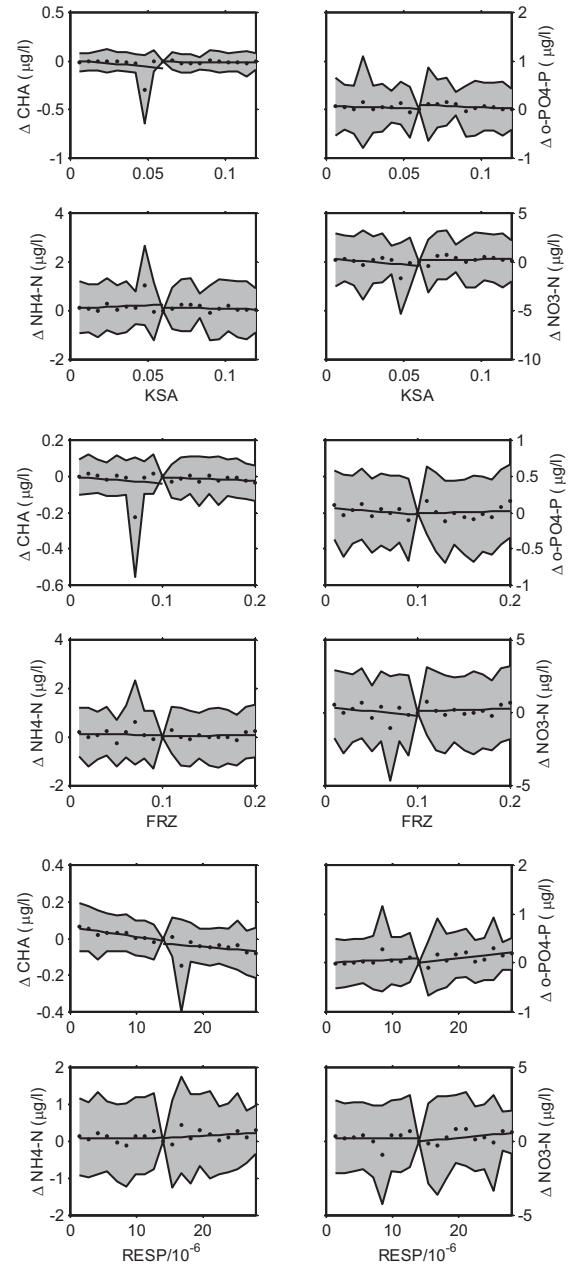


Figure 5 Sensitivity of variables CHA, o-PO₄-P, NH₄-N and NO₃-N to the parameters of group G3

Generally, for this group of parameters the variations of algal biomass are smaller than for variations of nutrients by changing parameter values. In the case of variations of KSA and FRZ the negative values of algal biomass follow the changes of the variable nitrate nitrogen. It can be derived that nitrogen is more dominant for algal growth concerning the Lower Havel River basin. In the case of parameter RESP both nutrients phosphorus and nitrogen have the same influence on algal growth.

5. CONCLUSIONS

Analysis of parameter sensitivity is an important task of the modelling procedure. Especially for complex systems like freshwater ecosystems these investigations are necessary to mark the parameter range of validity for environmental management decisions.

The output of the eutrophication simulator investigated is sensitive for parameter changes influencing phytoplankton growth. Another level of parameter sensitivity is given by parameters describing nutrient cycles and matter fluxes within the water body. In opposite of that, a constant influence of the variable zooplankton to phytoplankton was found. On the other hand, a higher influence of nitrogen to phytoplankton biomass compared with orthophosphate phosphorus could be derived from sensitivity analysis.

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